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Abstract

This paper is concerned with the numerical solution of the Boltzmann semiconductor equation. Our main objective is the development of a fast deterministic solution procedure for the numerical computation of the steady state solutions.

The discretization strategy is based on an upwind finite difference approximation of the gradient terms and on a deterministic conservative calculation of the integral operators. The resulting algebraic system is then solved by a least squares methodology which reduces the system to a quadratic minimization problem to be solved by a standard conjugate gradient algorithm.

L'EQUATION DE BOLTZMANN DES SEMICONDUCTEURS DANS LE CAS PERIODIQUE.

Résumé

On s'intéresse dans cet article à la résolution numérique de l'équation de Boltzmann des semiconducteurs. Notre but est de développer une méthode déterministe rapide pour le calcul numérique des solutions stationnaires.

La discrétisation repose sur une approximation par différences finies avec décentrage amont et sur un calcul conservatif déterministe des opérateurs intégraux. Le système algébrique qui en résulte est alors résolu par une méthodologie de moindres carrés qui se ramène à un problème de minimisation quadratique résolue par un algorithme de gradient conjugué standard.

Mots-clés: équation de Boltzmann, semiconducteurs, moindres carrés, intégrales de collision, différences finies décentrées.

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Introduction

This paper is concerned with the numerical solution of the Boltzmann semiconductor equation. Our main objective is the development of a fast deterministic solution procedure for the numerical computation of the steady state solutions.

In this framework, our discretization strategy is based on an upwind finite difference approximation of the gradient terms and on a deterministic conservative calculation of the integral operators. The resulting algebraic system is then solved by a least squares methodology which reduces the system to a quadratic minimization problem to be solved by a standard conjugate gradient algorithm.

In the axisymmetric steady case problem with periodic boundary conditions, this methodology gives nice results for all values of the electric fields. These results are confirmed by an unsteady analysis which, although more expensive numerically, gives additional information on the relaxation behavior of the distribution function towards its steady state. This situation is particularly well suited for semiconductor superlattices, which are periodic in the wavespace, with small periods in the direction of the electric field and large periods in the perpendicular direction ([1], [2]).

1. The Initial Problem

For the homogeneous problem in space, the semiconductor Boltzmann equation writes

$$\frac{\partial f}{\partial t} - \frac{q}{\hbar} E \cdot \nabla_k f = Q(f) \quad \text{in} \quad \mathbb{R}^3, \tag{1.1}$$

$$\int_{\mathbb{R}^3} f(k)dk = 1. \tag{1.2}$$

Here, the unknown f denotes the distribution of electron states k, q is the electric charge, E is the electric field and Q denotes the linear scattering operator given by

$$Q(f) = \int_{\mathbb{R}^3} (s(k';k)f(k') - s(k;k')f(k))dk'.$$

This operator can be decomposed into

$$Q(f) = S(f) - \frac{f}{\tau},$$

under the notation

$$S(f) = \int_{\mathbb{R}^3} s(k';k)f(k')dk' \quad \text{(scattering in)},$$

$$\frac{1}{\tau} = \int_{\mathbb{R}^3} s(k;k')dk' \quad \text{(scattering out)}.$$

In general, denoting by $\varepsilon(k)$ the energy versus wave-vector relation, the transmission rate $s(k',k)$ is a Dirac measure carried by the curves :

$$\varepsilon(k') = \varepsilon(k) \pm \hbar\omega_o,$$

and of intensity

$$(N_o + \frac{1}{2} \pm \frac{1}{2})d(k';k).$$

Above $\hbar w_o$ is the energy of the optical phonon and N_o is the number of phonons. Here, we have restricted ourselves to the case where the only scattering process is the polar optical phonon mode. Since d is a symmetric function of k and k', the above form of s implies that we have

$$s(k';k) = s(k;k')exp(\varepsilon(k') - \varepsilon(k)),$$

and thus the scattering kernel of Q is given by

$$\mathcal{N} = \{f, f(k) = \lambda exp(-\varepsilon(k)\}$$

and corresponds to the Maxwell-Boltzmann expression, which is valid for non interacting electrons.

Moreover, by construction, the scattering operator Q satisfies the identity

$$\int_{\mathbb{R}^3} Q(f)dk = \int\int_{\mathbb{R}^3\times\mathbb{R}^3} s(k';k)f(k')dk'dk - \int\int_{\mathbb{R}^3\times\mathbb{R}^3} s(k;k')f(k)dk'dk = 0,$$

implying the conservation of electric charges within the system under study.

Finally, recall that the stationary problem is simply obtained by removing the evolution term $\frac{\partial f}{\partial t}$ from the above Boltzmann equation (1.1).

2. Discretization Strategy

2.1. Finite Difference Approximation

By opposition to [3] or [4], our discretization strategy is based on an upwind finite difference approximation of the gradient terms and on a deterministic calculation of the integral operators.

We first begin by considering a problem *periodic* in the wave-vector k and *stationary* in time. This greatly simplifies the choice of a computational domain and of the corresponding boundary conditions. In such situations, the electric field is of direction k_z, the energy $\varepsilon(k)$ is supposed to be periodic in k_z of period K, and we look for an axisymmetric distribution $f(k_z, k_r)$ which is assumed to be stationary in time and periodic in k_z. Under these restrictions, the continuous problem takes the form

$$\begin{aligned}
&\text{Find} \quad f : D = [-\frac{K}{2}, \frac{K}{2}] \times [0, \infty) \rightarrow \mathbb{R} \quad \text{such that} \\
&\alpha \frac{\partial f}{\partial k_z} + \frac{f}{\tau} = S(f), \quad \forall M = (k_z, k_r) \in D, \\
&f(-\frac{K}{2}, k_r) = f(\frac{K}{2}, k_r), \quad \forall k_r > 0, \\
&\int_D 2\pi k_r f dk_r dk_z = 1,
\end{aligned}$$

under the notation $\alpha = -q|E|/\hbar$.

By further restricting the computational domain to the strip $D_h = (-\frac{K}{2}, \frac{K}{2}) \times (0, k_{rmax})$, by endowing this strip with a rectangular grid of vertices $\{k_{i,j}\}_{i=imin,imax;j=1,jmax}$, and by using an upwind finite difference approximation of the gradient $\alpha \frac{\partial f}{\partial z}$, this continuous problem can be approximated by the discrete system

$$\begin{aligned}
&\text{Find} \quad \{f_{i,j}\}_{i=imin,imax;j=1,jmax} \quad \text{such that} \\
&\alpha \frac{f_{i,j} - f_{i-1,j}}{z_i - z_{i-1}} + \frac{f_{i,j}}{\tau_{ij}} = (Sf)_{ij}, \quad \forall imin < i \leq imax, \quad \forall j, \\
&f_{imin,j} = f_{imax,j}, \quad \forall \quad 1 \leq j \leq jmax, \\
&\int_{D_h} 2\pi k_r f dk_r dk_z = 1,
\end{aligned}$$

under the obvious notation

$$f_{i,j} = f(k_{i,j}),$$

$$k_{i,j} = \{z_i, r_j\} = \quad \text{vertex} \quad \{i, j\} \quad \text{of the discretization grid.}$$

2.2. Deterministic Evaluation of the Integrals

In the above discrete problem, we have to compute the integrals

$$\int_{D_h} 2\pi k_r f dk_r dk_z,$$

$$(Sf)_{i,j} = \int_{\mathbb{R}^3} s(k'; k_{i,j}) f(k') dk'.$$

By taking into account the periodicity of f, the first integral can be evaluated by the classical quadrature rule

$$\int_{D_h} 2\pi k_r f dk_r dk_z = 2\pi \sum_{i=imin+1}^{imax} \sum_{j=1}^{jmax} r_j h_{zi} h_{rj} f_{i,j} \tag{2.1}$$

with

$$h_{zi} = (z_{i+1} - z_{i-1})/2 \quad \text{if} \quad imin < i < imax,$$

$$h_{zimax} = \frac{1}{2}(z_{imin+1} + z_{imax} - z_{imin} - z_{imax-1}),$$

$$h_{rj} = (r_{j+1} - r_{j-1})/2.$$

For the second integral, due to the periodicity of f, we have

$$\int_{\mathbb{R}^3} s(k'; k_{i,j}) f(k') dk' = \int_D \sum_{p \in \mathbb{Z}} s(k' + pK; k_{i,j}) f(k') 2\pi k'_r dk'_r dk'_z$$

$$\approx \int_{D_h} \sum_{p \in \mathbb{Z}} s(k' + pK; k_{i,j}) f(k') 2\pi k'_r dk'_r dk'_z.$$

To be consistent with the computation of the first integral, and also by analogy with the particle approach of [3], [4], we have chosen to replace the Dirac measure s by a regular approximating function s_b and to integrate the resulting integral by the quadrature rule (2.1) used for the first integral.

We therefore obtain

$$\int_{\mathbb{R}^3} s(k'; k_{i,j}) f(k') dk' \approx \sum_{k>imin} \sum_{l} (\sum_{p \in \mathbb{Z}} s_b(k_{k,l} + pK; k_{i,j})) f_{k,l} 2\pi r_l h_{zk} h_{rl}, \tag{2.2}$$

$$\approx \sum_{k>imin} \sum_{l} S_{ijkl} f_{k,l},$$

under the notation

$$S_{ijkl} = (\sum_{p \in \mathbb{Z}} s_b(k_{k,l} + pK; k_{i,j}) 2\pi r_l h_{zk} h_{rl}. \tag{2.3}$$

In practice, the calculation of the term between brackets is done as follows (cf. fig. 1) :
i) we first compute a cut-off parameter b by

$$b = b_o sup(1, \sqrt{\varepsilon(k_{i,j})}/2), \quad b_o \geq 2h;$$

ii) we then define the cut-off function δ_b ([5]) by

$$\delta_b(x) = sup[\frac{2}{b} - \frac{4|x|}{b^2}, 0];$$

iii) for each $k_{i,j}$, we also define the four points

$$\{k^r_{i,j}\}_{r=1,4} = \{z_i \pm \frac{h}{2}, r_j \pm \frac{h}{2}\};$$

iv) we finally set

$$(2.4) \quad \sum_{p\in\mathbf{Z}} s_b(k_{k,l} + pK; k_{i,j}) = \sum_{p\in\mathbf{Z}} \sum_{r=1}^{4} \sum_{s=1}^{4} \sum_{t=1}^{2} \frac{1}{16}(N_o + \frac{1}{2} + \frac{(-1)^t}{2}) d(k^r_{k,l} + pK; k^s_{i,j}) \times$$

$$\times \delta_b(\varepsilon(k^r_{k,l}) - \varepsilon(k^s_{i,j}) + (-1)^t \hbar\omega_o).$$

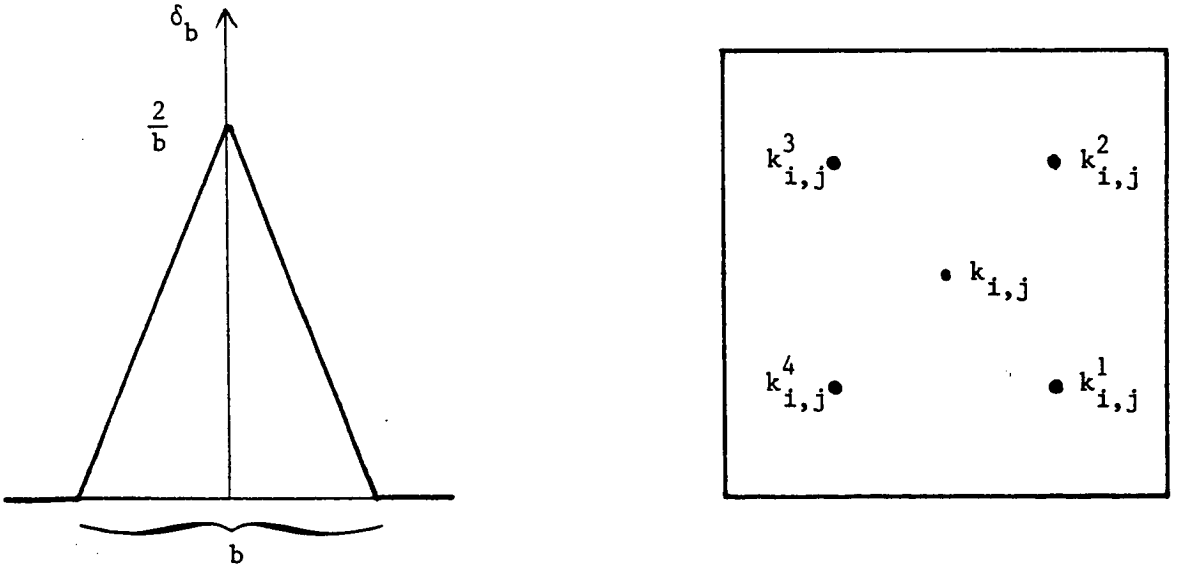


Figure 1

In this calculation, we regularize the transition rate both by replacing the Dirac measure by the cut-off function δ_b and by averaging the result on different perturbed positions

of the "particles" $k_{i,j}$ and $k_{k,l}$. Moreover, because of the fast decrease of d with the difference $|k_{k,l} - k_{i,j}|$, the summation on p is not carried on $\mathbf{Z}$ but on intervals of the type $\{-q, q\}$ with $q \leq 4$. Figure 2 shows the aspect and the large singularities of S_{ijkl}.

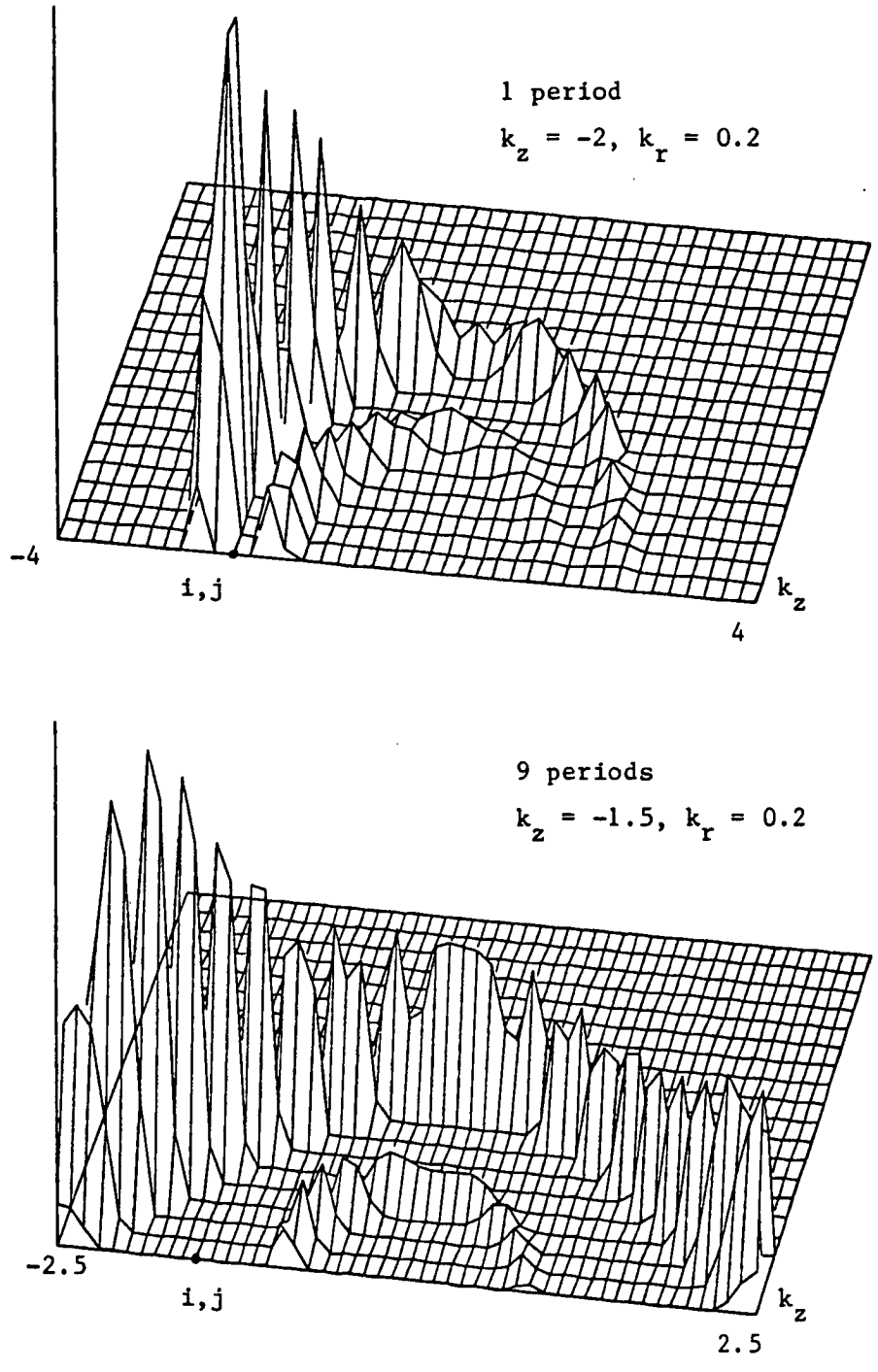


Figure 2 : Aspects of $k, l \rightarrow S_{ijkl}$

2.3. Evaluating the collision frequency

The calculation of $\frac{1}{\tau}$ could be done by using the quadrature rule already used for computing Sf. This turns out to be a very bad numerical choice. Indeed, the round-off and truncation errors involved in these quadrature rules will lead to slightly inconsistent values of $\frac{f}{\tau}$ and of Sf, resulting in discrete solutions with locally negative values. These negative values, however very small (10^{-5} or less), will affect strongly the values of the computed averages :

$$< v >= \int_D v_{k_z} f(k)dk, \quad \text{with} \quad v_{k_z} = \frac{1}{\hbar}\nabla_k \varepsilon(k),$$

$$< \mathcal{E} >= \int_D \varepsilon(k) f(k)dk.$$

To avoid such accidents with this strategy, one must then be extremely accurate, consistent and careful in the choice of the cut-off functions and of the quadrature weights. This leads therefore to expensive numerical computations.

A better idea is to compute $\frac{1}{\tau}$ not by evaluating the corresponding integral but by imposing that the conservation properties which are satisfied at the continuous level still hold at the discrete level. More precisely, by definition of $\frac{f}{\tau}$ and of Sf, we have, for any distribution function f,

$$\int_{\mathbb{R}^3} \frac{1}{\tau} f(k)dk = \int_{\mathbb{R}^3 \times \mathbb{R}^3} s(k;k') f(k)dkdk'$$

$$= \int_{\mathbb{R}^3 \times \mathbb{R}^3} s(k';k) f(k')dk'dk$$

$$= \int_{\mathbb{R}^3} dk \int_{\mathbb{R}^3} s(k';k) f(k')dk'dk$$

$$= \int_{\mathbb{R}^3} Sf dk.$$

After discretization over m periods, the first integral is to be appoximated by

$$\int_{\mathbb{R}^3} \frac{1}{\tau} f(k) \approx m \int_{D_h} \frac{1}{\tau} f(k)dk \approx m \sum_{i=imin+1}^{imax} \sum_{j=1}^{jmax} 2\pi r_j h_{zi} h_{rj} \frac{f_{i,j}}{\tau_{ij}}.$$

As for the second integral, it comes

$$\int_{\mathbb{R}^3} Sf dk \approx m \sum_{k=imin+1}^{imax} \sum_{l=1}^{jmax} 2\pi r_l h_{zk} h_{rl} (Sf)_{kl},$$

that is, replacing $(Sf)_{kl}$ by the value computed in (2.2),

$$\int_{\mathbb{R}^3} Sf dk \approx m \sum_{k=imin+1}^{imax} \sum_{l=1}^{jmax} \sum_{i=imin+1}^{imax} \sum_{j=1}^{jmax} 2\pi r_l h_{zk} h_{rl} S_{klij} f_{i,j}.$$

Imposing that these two integrals stay equal after discretization, this for any distribution function f, leads to the condition

$$\frac{1}{\tau_{ij}} = \frac{1}{r_j h_{zi} h_{rj}} \sum_{k=imin+1}^{imax} \sum_{l=1}^{jmax} r_l h_{zk} h_{rl} S_{klij}. \tag{2.5}$$

This formula turns out to be the best way of computing $\frac{1}{\tau_{ij}}$.

2.4. The discrete formulation of the stationary periodic problem

We now derive the discrete formulation of the *stationary problem* in the k *periodic* case. Using the finite difference approximation derived above together with the numerical quadratures just proposed for computing the different integrals, we get

$$\text{Find} \quad \{f_{i,j}\}_{i=imin,imax,j=1,jmax} \quad \text{such that}$$

$$\alpha \frac{f_{i,j} - f_{i-1,j}}{z_i - z_{i-1}} + \frac{1}{\tau_{i,j}} f_{i,j} = \sum_{k=imin+1}^{imax} \sum_{l=1}^{jmax} S_{ijkl} f_{k,l}, \tag{2.6}(i)$$

$$\forall imin < i \leq imax, \quad \forall j = 1, jmax,$$

$$f_{imin,j} = f_{imax,j}, \quad \forall j = 1, jmax, \tag{2.7}(ii)$$

$$\sum_{i=imin+1}^{imax} \sum_{j=1}^{jmax} 2\pi r_j h_{zi} h_{rj} f_{i,j} = 1, \tag{2.8}(iii)$$

with S_{ijkl} and τ_{ij} given by (2.3) and (2.5) respectively.

As written, this is a large linear system associated to a rectangular unsymmetric matrix. As such, its solution by a direct method is costly and difficult.

2.5. The discrete formulation of the evolution problem

The only change between the stationary and the evolution problem concerns the transport operator $\alpha \frac{\partial f}{\partial k_z}$ which now writes

$$T f = \frac{\partial f}{\partial t} + \alpha \frac{\partial f}{\partial k_z}.$$

If we use an implicit time discretization of the evolution term $\frac{\partial f}{\partial t}$, the discrete problem is then transformed into the sequence of problems

With $\{f_{i,j}^{n-1}\}$ *known, find* $\{f_{i,j}^{n}\}$ *such that*

$$(2.9)(i) \qquad \frac{f_{i,j}^{n} - f_{i,j}^{n-1}}{\Delta t} + \alpha \frac{f_{i,j}^{n} - f_{i-1,j}^{n}}{z_i - z_{i-1}} + \frac{1}{\tau_{ij}} f_{i,j}^{n} = \sum_{k>imin} \sum_{l} S_{ijkl} f_{k,l}^{n},$$

$$\forall imin < i \leq imax, \quad \forall 1 \leq j \leq jmax,$$

$$(2.10)(ii) \qquad f_{imin,j}^{n} = f_{imax,j}^{n}, \quad \forall 1 \leq j \leq jmax,$$

$$(2.11)(iii) \qquad \sum_{i>imin} \sum_{j} 2\pi r_j h_{zi} h_{rj} f_{i,j}^{n} = 1.$$

If we use an implicit discretization along the characteristics of T, the discrete problem becomes

With $\{f_{i,j}^{n-1}\}$ *known, find* $\{f_{i,j}^{n}\}$ *such that*

$$(2.12)(i) \qquad \frac{f_{i,j}^{n} - f_{i-\alpha\Delta t,j}^{n-1}}{\Delta t} + \frac{1}{\tau_{ij}} f_{i,j}^{n} = \sum_{k>imin} \sum_{l} S_{ijkl} f_{k,l}^{n},$$

$$(2.13)(ii) \qquad f_{imin,j}^{n} = f_{imax,j}^{n}, \quad \forall 1 \leq j \leq jmax,$$

$$(2.14)(iii) \qquad \sum_{i>imin} \sum_{j} 2\pi r_j h_{zi} h_{rj} f_{i,j}^{n} = 1.$$

Here, $f_{i-\alpha\Delta t,j}$ denotes the approximation of f at point $\{z_i - \alpha\Delta t, r_j\}$.

In both situations, due to the conservation property (2.5), the normalization constraints (2.11) or (2.14) are automatically satisfied by the solutions of (2.9)-(2.10) or of (2.12)-(2.13), provided that these constraints are satisfied at step $(n-1)$. Therefore, these two constraints can be completely dropped.

2.6. The discrete formulation of the stationary unbounded problem

The situation is more complex if the Boltzmann equation is to be solved on the *whole space* $\mathbb{R}^3$. To obtain a bounded computational domain, a first solution is to approximate this problem by a periodic one, of period $[-k_{zmax}, k_{zmax}]$. If k_{zmax} is sufficiently large, it is hoped that such periodic boundary conditions will mimick the unbounded case where

the solution is to decrease to zero at infinity. With this choice, we can keep the previous discrete formulation.

A second solution truncates $\mathbb{R}^3$ to the same computational domain $D = [-k_{zmax}, k_{zmax}] \times \mathbb{R}^2$ but replaces the periodic boundary conditions by the "upwind" Dirichlet condition

$$f(-k_{zmax}, k_r) = 0, \quad \forall k_r \geq 0.$$

As a consequence, all summations on i, which, due to periodicity, were only carried from $imin+1$ to $imax$, must now be carried from $imin$ to $imax$. Then, our previous discretization strategy now leads to the problem

$$\text{Find} \quad \{f_{i,j}\}_{i=imin,imax,j=1,jmax} \quad \text{such that}$$

(2.14)(i)
$$\alpha \frac{f_{i,j} - f_{i-1,j}}{z_i - z_{i-1}} + \frac{f_{i,j}}{\tau_{i,j}} = \sum_{i=imin}^{imax} S_{ijkl} f_{k,l}, \quad \forall i > imin, \quad \forall j,$$

(2.15)(ii)
$$f_{imin,j} = 0, \quad \forall j = 1, jmax,$$

(2.16)(iii)
$$\sum_{i=imin}^{imax} \sum_{j=1}^{jmax} 2\pi r_j h_{zi} h_{rj} f_{i,j} = 1,$$

with

$$S_{ijkl} = 2\pi r_l h_{zk} h_{rl} s_b(k_{k,l}, k_{i,j}),$$

$$\frac{1}{\tau_{i,j}} = \sum_{k=imin}^{imax} \sum_{l=1}^{jmax} \frac{r_l}{r_j} \frac{h_{zk}}{h_{zi}} \frac{h_{rl}}{h_{rj}} S_{klij}.$$

3. Numerical Algorithm

3.1. Least squares formulation

We again begin by considering the stationary case with periodic boundary conditions. Then, the discrete formulation of Par. 2 takes the abstract from :

$$\begin{cases} T_h f = S_h f, \\ f \in V_h^1, \end{cases}$$

with

$$V_h^1 = \{v = \{v_{i,j}\}, \quad L(v) = 1\},$$

$$L(v) = (v, 1),$$

$$(v,w) = \sum_{ij} 2\pi r_j h_{zi} h_{rj} v_{i,j} w_{i,j},$$

(3.1) $$(S_h v)_{ij} = \sum_{kl} S_{ijkl} v_{k,l} = \quad \text{"source" term},$$

(3.2) $$(T_h v)_{ij} = \alpha \frac{v_{i,j} - v_{imax,j}}{z_i - z_{i-1}} + \frac{v_{i,j}}{\tau_{i,j}} \quad \text{if} \quad i = imin + 1,$$

$$= \alpha \frac{v_{i,j} - v_{i-1,j}}{z_i - z_{i-1}} + \frac{v_{i,j}}{\tau_{i,j}} \quad \text{if} \quad imin + 1 < i \leq imax.$$

Herein, the indices i and k are restricted to the interval $\{imin + 1, imax\}$.

Provided that there exists a solution, this problem is clearly equivalent to the least squares problem

(3.3) $$J(u) \leq J(v), \quad \forall v \in V_h^1, \quad u \in V_h^1,$$

if we set

$$J(v) = \frac{1}{2}\|v - Av\|^2,$$

$$Av = T_h^{-1} S_h v,$$

$$\|w\|^2 = (\chi w, \chi w),$$

with χ an arbitrary weight function. Denoting by V_h^o the kernel of L, the least squares problem (3.3) writes

$$(\nabla J(u), v) = 0, \quad \forall v \in V_h^o, \quad u \in V_h^1.$$

This linear variational problem can now be solved by the following classical conjugate gradient algorithm ([6]) :

Initialization. With $u^o \in V_h^1$ given,
- compute $g^o = \nabla J(u^o)$,
- set $w^o = g^o$.

Step 1. Descent. With u^n, g^n and w^n known,
- compute $z^n = \nabla J(w^n)$,
- set $\rho_n = (g^n, w^n)/(z^n, w^n)$,
- set $u^{n+1} = u^n - \rho_n w^n$,
- set $g^{n+1} = g^n - \rho_n z^n$,
- set $\varepsilon_n = (g^{n+1}, g^{n+1})/(g^o, g^o)$.

If $\varepsilon^n \leq 10^{-5}$, then $f = T_h^{-1} S_h u^{n+1}$, otherwise we go to step 2.

Step 2. New descent direction.
• set $\gamma_{n+1} = (g^{n+1}, g^{n+1})/(g^n, g^n)$,
• set $w^{n+1} = g^{n+1} + \gamma_{n+1} w^n$,
and return to step 1.

3.2. Computing the gradient of J

This is one of the key points of the proposed numerical method. For efficiency reasons, this calculation must be fast and accurate. By definition, we have :

$$J(v) = \frac{1}{2}(\chi(v - Av), \chi(v - Av)),$$

from which we deduce

$$(\nabla J(v), w) = (\chi(v - Av), \chi(w - Aw)), \quad \forall w \in V_h^o, \quad \nabla J \in V_h^o.$$

Introducing the state vector $y = Av$, and the adjoint state

$$p = A^T \chi^2 (v - y)$$

to be computed later, this characterization of ∇J writes

$$(\nabla J(v), w) = (\chi^2(v - y), w) - (A^T \chi^2 (v - y), w)$$

$$= (\chi^2(v - y) - p, w), \quad \forall w \in V_h^o, \quad \nabla J \in V_h^o.$$

Introducing now the Lagrange multiplier of the constraint $L(\nabla J) = (1, \nabla J) = 0$, this system can be rewritten as

$$\begin{cases} (\nabla J(v), w) = (\chi^2(v - y) - p, w) - \lambda(1, w), & \forall w, \\ (1, \nabla J) = 0, \end{cases}$$

which means that we finally have

$$\nabla J(v) = \chi^2(v - y) - p - \frac{(1, \chi^2(v - y) - p)}{(1, 1)} 1. \tag{3.4}$$

3.3. Computing the state vector and the adjoint state

In the case of periodic boundary conditions, the state vector $y = Av = T_h^{-1} S_h v$ satisfies

$$T_h y = S_h v,$$

that is

(3.5) $$\alpha\frac{y_{i,j}-y_{i-1,j}}{z_i-z_{i-1}}+\frac{y_{i,j}}{\tau_{i,j}}=\sum_{k>imin}\sum_{l}S_{ijkl}v_{k,l}$$

$$\forall\, imin<i\leq imax,\quad \forall\, 1\leq j\leq jmax,$$

with $y_{i-1,j}$ replaced by $y_{imax,j}$ if $i=imin+1$.

For a given j, this is a linear system with matrix structure

$$T=\begin{bmatrix} \bullet & & & & & & \bullet \\ \bullet & \bullet & & & & & \\ & \bullet & \bullet & & & & \\ & & \bullet & \bullet & & & \\ & & & \bullet & \bullet & & \\ & & & & \bullet & \bullet & \\ & & & & & \bullet & \bullet \end{bmatrix}.$$

As such it can be solved in three steps (block Gauss elimination) :

i) two forward substitutions to express $y_{i,j}$ in function of $y_{imax,j}$ and $S_h v$;

ii) the solution of the scalar equation in $y_{imax,j}$;

iii) one forward substitution starting from the computed value of $y_{imax,j}$ to get the final values of $y_{i,j}$.

These operations can be done in parallel on j, which can lead to interesting speed-ups on vector or parallel machines.

To compute $A^T v$, we first have to compute $q=T_h^{-T}v$, that is to solve

$$(q,T_h w)=(v,w),\quad \forall w.$$

By definition of the scalar product, this writes

$$\sum_{i,j}2\pi r_j h_{zi}h_{rj}[\alpha\frac{w_{i,j}-w_{i-1,j}}{z_i-z_{i-1}}+\frac{w_{i,j}}{\tau_{ij}}]q_{i,j}=$$

$$+\sum_{i,j}2\pi r_j h_{zi}h_{rj}v_{i,j}w_{i,j},\quad \forall w,$$

with $w_{i-1,j}$ replaced by $w_{imax,j}$ if $i=imin+1$. By grouping together the terms in $w_{i,j}$, this equation can be rewritten as

$$0=\sum_j 2\pi r_j h_{rj}\sum_i w_{i,j}[h_{zi}q_{i,j}(\frac{\alpha}{z_i-z_{i-1}}+\frac{1}{\tau_{i,j}})-\alpha\frac{h_{zi+1}q_{i+1,j}}{z_{i+1}-z_i}-h_{zi}v_{i,j}].$$

By cancelling all the coefficients in $w_{i,j}$, we finally obtain that $q = T_h^{-T} v$ is solution of the linear system

$$h_{zi} q_{i,j} \left(\frac{\alpha}{z_i - z_{i-1}} + \frac{1}{\tau_{i,j}} \right) - \alpha \frac{h_{zi+1} q_{i+1,j}}{z_{i+1} - z_i} = h_{zi} v_{i,j}, \tag{3.6}$$

$$\forall imin < i \leq imax, \forall 1 \leq j \leq jmax.$$

Here, because of the identification $w_{imin,j} = w_{imax,j}$, the term $\frac{h_{zi+1} q_{i+1,j}}{z_{i+1} - z_i}$ has to be replaced by $\frac{h_{zimin+1} q_{imin+1,j}}{z_{imin+1} - z_{imin}}$ when $i = imax$. The resulting system in q has then the same structure as the previous system in y and is therefore as easy to solve.

Once q computed, we directly have

$$\begin{aligned}
(A^T v, w) &= (v, Aw) \\
&= (q, T_h A w) \\
&= (q, S_h w) \\
&= \sum_{ijkl} 2\pi r_j h_{zi} h_{rj} q_{i,j} S_{ijkl} w_{k,l} \\
&= \sum_{kl} 2\pi r_l h_{zk} h_{rl} w_{k,l} \left(\sum_{ij} \frac{r_j h_{zi} h_{rj}}{r_l h_{zk} h_{rl}} S_{ijkl} q_{i,j} \right)
\end{aligned}$$

and hence, after identification,

$$(A^T v)_{kl} = \sum_{ij} \frac{r_j h_{zi} h_{rj}}{r_l h_{zk} h_{rl}} S_{ijkl} q_{i,j}. \tag{3.7}$$

In summary, for the stationary problem with periodic boundary conditions, the computation of the gradient of J amounts to

i) computing $y = Av$ by solving (3.5) ;
ii) computing $q = T_h^{-T}(\chi^2(v - y))$ by solving (3.6) with v replaced by $\chi^2(v - y)$;
iii) computing $p = A^T(\chi^2(v - y))$ by (3.7) ;
iv) computing ∇J by (3.4).

3.4. The evolution problem

For the periodic evolution problem, the discrete formulations (2.9)-(2.10) or (2.12)-(2.13) take the abstract form

$$T_h f^n = S_h f^n + \frac{f^{n-1}}{\Delta t}.$$

For the case of the implicit discretization in time (2.9)-(2.10), S_h is given by (3.1) and we have :

$$(T_h v)_{ij} = \alpha \frac{v_{i,j} - v_{imax,j}}{z_i - z_{i-1}} + (\frac{1}{\Delta t} + \frac{1}{\tau_{i,j}}) v_{i,j} \quad \text{if} \quad i = imin + 1,$$

$$= \alpha \frac{v_{i,j} - v_{i-1,j}}{z_i - z_{i-1}} + (\frac{1}{\Delta t} + \frac{1}{\tau_{i,j}}) v_{i,j} \quad \text{if} \quad imin + 1 < i \leq imax,$$

$$(f^{n-1}/\Delta t)_{ij} = f^{n-1}_{i,j}/\Delta t.$$

For the case of problem (2.12)-(2.13) (discretization along characteristics), S_h is given by (3.1) and we have

$$(T_h v)_{i,j} = (\frac{1}{\Delta t} + \frac{1}{\tau_{i,j}}) v_{i,j},$$

$$(\frac{f^{n-1}}{\Delta t})_{i,j} = \frac{f^{n-1}_{i-\alpha \Delta t,j}}{\Delta t}.$$

With these definitions, our least squares problem now becomes

$$J(f^n) \leq J(v), \quad \forall v,$$

with J given by

$$J(v) = \frac{1}{2} \| v - T_h^{-1}(S_h v + \frac{f^{n-1}}{\Delta t}) \|^2.$$

This problem can again be solved by the conjugate gradient algorithm of §3.1. Nevertheless, the calculation of ∇J will be simpler here because we have dropped the normality constraint $(L, v) = 1$. More precisely, under the notations of §3.1 and §3.2, we have simply

$$\nabla J(v + dv) = \nabla J(v) + \chi^2(dv - dy) - dp,$$

with dy and dp computed as in §3.3 within the replacement of $\frac{1}{\tau_{i,j}}$ by $(\frac{1}{\tau_{i,j}} + \frac{1}{\Delta t})$ (and the replacement of α by 0 if we are using the formulation (2.12)-(2.13)).

3.5. The stationary Dirichlet problem

In this case, the discrete formulation (2.14)-(2.16) takes the abstract form

$$\begin{cases} T_h f = S_h f, \\ f \in V^1_{0h}, \end{cases}$$

under the new notation

$$V^1_{0h} = \{v = \{v_{i,j}\}, \quad L(v) = 1, \quad v_{imin,j} = 0\},$$

$$(T_h v)_{i,j} = \alpha \frac{v_{i,j} - v_{i-1,j}}{z_i - z_{i-1}} + \frac{v_{i,j}}{\tau_{ij}}, \quad \forall imin < i \leq imax.$$

In this section, unless explicitly specified, the indices i and k span the whole interval $\{imin, imax\}$. Within this correction, the definitions of $S_h, L(\cdot,\cdot)$ and $\|\cdot\|$ are those of §3.1.

If we treat the artificial boundary condition $v_{imin,j} = 0$ by a penalization technique, the above abstract problem can be transformed into the least squares problem

$$J(f,\eta) \leq J(v,\xi), \quad \forall \{v,\xi\} \in W_h^1, \{f,\eta\} \in W_h^1,$$

under the notation

$$J(v,\xi) = \frac{1}{2}\|v - A(v,\xi)\|^2 + \frac{\beta}{2}\xi \cdot \xi,$$

$$W_h^1 = \{\{v,\xi\} = \{v_{i,j}, \xi_j\}, \quad L(v) = 1\},$$

$$\xi \cdot \eta = \sum_j 2\pi r_j h_{rj} \xi_j \eta_j.$$

Above, $y = A(v,\xi)$ denotes the solution of the linear triangular systems (one for each j)

$$\text{(3.8)} \qquad \begin{cases} \alpha \dfrac{y_{i,j} - y_{i-1,j}}{z_i - z_{i-1}} + \dfrac{y_{i,j}}{\tau_{i,j}} = \displaystyle\sum_{kl} S_{ijkl} v_{k,l}, \quad \forall i > imin, \\ y_{imin,j} = \xi_j. \end{cases}$$

This least squares problem is solved by our previous conjugate gradient algorithm operating on $W_h^o = KerL$ that we endow with the scalar product

$$[\{v,\xi\},\{w,\eta\}] = (v,w) + \xi \cdot \eta.$$

Computing the gradient of J for this scalar product is again a basic and technical step of this algorithm. For this, we must solve

$$[\nabla J, \{w,\eta\}] = (\chi(v - A(v,\xi)), \chi(w - A(w,\eta))) + \beta\xi \cdot \eta.$$

$$\forall \{w,\eta\} \in W_h^o, \quad \{w,\xi\} \in W_h^o.$$

To compute the right hand side of this equation, we proceed as in Par. 3.3 and first compute q by solving the triangular system

$$\text{(3.9)} \qquad \begin{cases} h_{zi} q_{i,j} \left(\dfrac{\alpha}{z_i - z_{i-1}} + \dfrac{1}{\tau_{i,j}}\right) - \alpha \dfrac{h_{zi+1} q_{i+1,j}}{z_{i+1} - z_i} = h_{zi} \chi_{ij}^2 (v - y)_{i,j}, \\ \forall imin \leq i < imax, \\ q_{imax,j} \left(\dfrac{\alpha}{z_{imax} - z_{imax-1}} + \dfrac{1}{\tau_{imax,j}}\right) = \chi_{imax,j}^2 (v - y)_{imax,j}. \end{cases}$$

We then have, with obvious notation,

$$(\chi^2(v-y), A(w,\eta)) = \sum_{i,j} 2\pi r_j h_{zi} h_{rj} \chi^2_{ij}(v-y)_{i,j} A_{i,j}$$

$$= \sum_j \sum_{i<imax} 2\pi r_j h_{rj} A_{i,j} (h_{zi} q_{i,j} [\frac{\alpha}{z_i - z_{i-1}} + \frac{1}{\tau_{i,j}}] - \alpha \frac{h_{zi+1} q_{i+1,j}}{z_{i+1} - z_i})$$

$$+2\pi \sum_j r_j h_{rj} A_{imax,j} q_{imax,j} [\frac{\alpha}{z_{imax} - z_{imax-1}} + \frac{1}{\tau_{imax,j}}]$$

$$= \sum_j \sum_{i>imin} 2\pi r_j h_{zi} h_{rj} q_{i,j} (\alpha \frac{A_{i,j} - A_{i-1,j}}{z_i - z_{i-1}} + \frac{A_{i,j}}{\tau_{i,j}})$$

$$+ \sum_j 2\pi r_j h_{rj} h_{zimin} A_{imin,j} q_{imin,j} [\frac{\alpha}{z_{imin} - z_{imin-1}} + \frac{1}{\tau_{imin,j}}]$$

$$= \sum_{i>imin} \sum_{jkl} 2\pi r_j h_{zi} h_{rj} q_{i,j} S_{ijkl} w_{k,l} +$$

$$+ \sum_j 2\pi r_j h_{zimin} \xi_j q_{imin,j} [\frac{\alpha}{z_{imin} - z_{imin-1}} + \frac{1}{\tau_{imin,j}}].$$

Plugging this in the right hand side of the equation in ∇J, and proceeding as in §3.2, we finally obtain

$$\nabla J = \{\nabla J_{ij}, \nabla J_{\xi j}\},$$

$$\nabla J_{ij} = \chi^2_{ij}(v_{i,j} - y_{i,j}) - p_{i,j} - \frac{(\chi^2(v-y) - p, 1)}{(1,1)} 1,$$

$$\nabla J_{\xi j} = h_{zimin} q_{imin,j} [\frac{\alpha}{z_{imin} - z_{imin-1}} + \frac{1}{\tau_{imin,j}}] + \beta \xi_j.$$

Here y denotes the solution of (3.8), q the solution of (3.9) and p is given by

$$p_{kl} = \sum_j \sum_{i>min} \frac{r_j h_{rj} h_{zi}}{r_l h_{rl} h_{zl}} S_{ijkl} q_{i,j}.$$

Once the gradient of J computed, the conjugate gradient algorithm can proceed without any further difficulty.

4. Numerical results

4.1. Notations and data

In our numerical tests, we have used the notation :

nit = number of iterations of the conjugate gradient algorithm,

$$\int f = 2\pi \sum_{i=imin}^{imax} \sum_{j=1}^{jmax} r_j h_{zi} h_{rj} f_{i,j}$$

$$\text{cost} = \begin{cases} \frac{1}{2}\|f - A(f)\|^2 & \text{(periodic problem),} \\ \frac{1}{2}\|f - A(f,\eta)\|^2 + \frac{\beta}{2}\eta \cdot \eta & \text{(Dirichlet problem).} \end{cases}$$

Moreover, the mean velocity and energy are respectively given by

$$< v >= \int_{D_h} v_k f(k) dk = 2\pi \sum_{i=i_o}^{imax} \sum_{j=1}^{jmax} r_j h_{zi} h_{rj} v_{zi} f_{i,j}$$

$$< \mathcal{E} >= \int_{D_h} \varepsilon(k) f(k) dk = 2\pi \sum_{i=i_o}^{imax} \sum_{j=1}^{jmax} r_j h_{zi} h_{rj} \varepsilon(k_{ij}) f_{i,j},$$

where $i_o = imin + 1$ for the periodic problem and $i_o = imin$ for the Dirichlet problem.

In addition, to assess the quality of our numerical solutions, we will monitor the numerical values of

$\lambda_1 =$ smallest eigenvalue of the operator $T_h - S_h$,

$\bar{\lambda} = \frac{1}{mes(D_h)} \int \nabla J(f) =$ multiplier of the constraint $\int f = 1$.

In the case of an efficient discretization strategy, one should obtain very small values of λ_1 (to be computed in the evolution problem) and should satisfy the relation

$$\bar{\lambda} = 0(\lambda_1^2).$$

For the periodic problems, the physical data are those of a semiconductor superlattice of $GaAs/AlAs$ type. The energy relation is given by

$$\varepsilon(k) = k_r^2 + \frac{\Delta}{2}(1 - cos(k_z d))$$

with $\Delta = 4$ = minibandwidth. The energy of the optical phonons is $\hbar\omega_o = 1.55$. All physical data are normalized in U_T units with $U_T = k_B T$, k_B the Boltzmann constant and T the absolute temperature. Similarly, the effective mass is normalized to 1. Finally, under the notation of Par. 1, the function $d(k, k')$ is always given by

$$d(k, k') = \gamma / [(k_r^2 - k_r'^2)^2 + (k_z - k_z')^4 + 2(k_z - k_z')^2 (k_r^2 + k_r'^2)]^{\frac{1}{2}},$$

with γ a constant depending only on the considered material.

Concerning the numerical parameters, we have taken $\chi = 1$ for the periodic problem and $\beta = 0.1$ and $\chi = max(1, \epsilon(k)^{\frac{1}{2}})$ for the Dirichlet problem. For steady state computations, the conjugate gradient algorithm is initialized by the constant function

$$f = [meas(D_h)]^{-1}.$$

4.2. The stationary periodic problem

4.2.1. The model problem. Here, we have :
$D_h = (-2.5, 2.5) \times (0, 4)$,
$h_z = 0.1, \quad h_r = 0.2$ (1020 unknowns),
$b_o = 0.4$ (reference cut-off parameter),
9 periods for computing S.

The corresponding results are summarized in Table 1. Figure 3 describes the aspect of f as function of the electric field : the distribution function is first shifted until α reaches 2, and then collapses towards a rather uniform distribution.

The number of iterations required for convergence is insensitive to the initialization procedure (constant, Maxwellian ...).

Each iteration lasts $2s$ on the CCVR Cray 2.

α	<v>	<ε>	$\bar{\lambda}$	nit	cost	$\int f$
0	0	1.626	-0.35E-7	64	0.19E-13	1.0001
0.5	0.394	1.737	0.13E-7	43	0.91E-14	1.0000
1	0.603	1.927	0.11E-7	37	0.37E-14	"
2	0.761	2.357	-0.79E-9	28	0.41E-14	"
3	0.767	2.745	-0.32E-8	25	0.48E-15	"
4	0.720	3.054	-0.79E-10	22	0.10E-14	"
5	0.657	3.289	0.29E-9	21	0.14E-15	"
6	0.596	3.465	0.22E-10	20	0.10E-15	"
8	0.493	3.699	-0.74E-9	18	0.21E-15	"
10	0.415	3.838	0.24E-9	18	0.63E-16	"

Table 1

4.2.2. Influence of the number of periods

We consider the same numerical test but now the computation of S uses $1, 2, 3$ or 7 periods. We observe that this number of periods has no influence on the numerical behavior of the algorithm $(nit, \int f, cost, \bar{\lambda})$. On the other hand, the mean velocity and energy are sensitive to this choice, and reach their asymptotic values when this number is greater than 7 (Fig. 4).

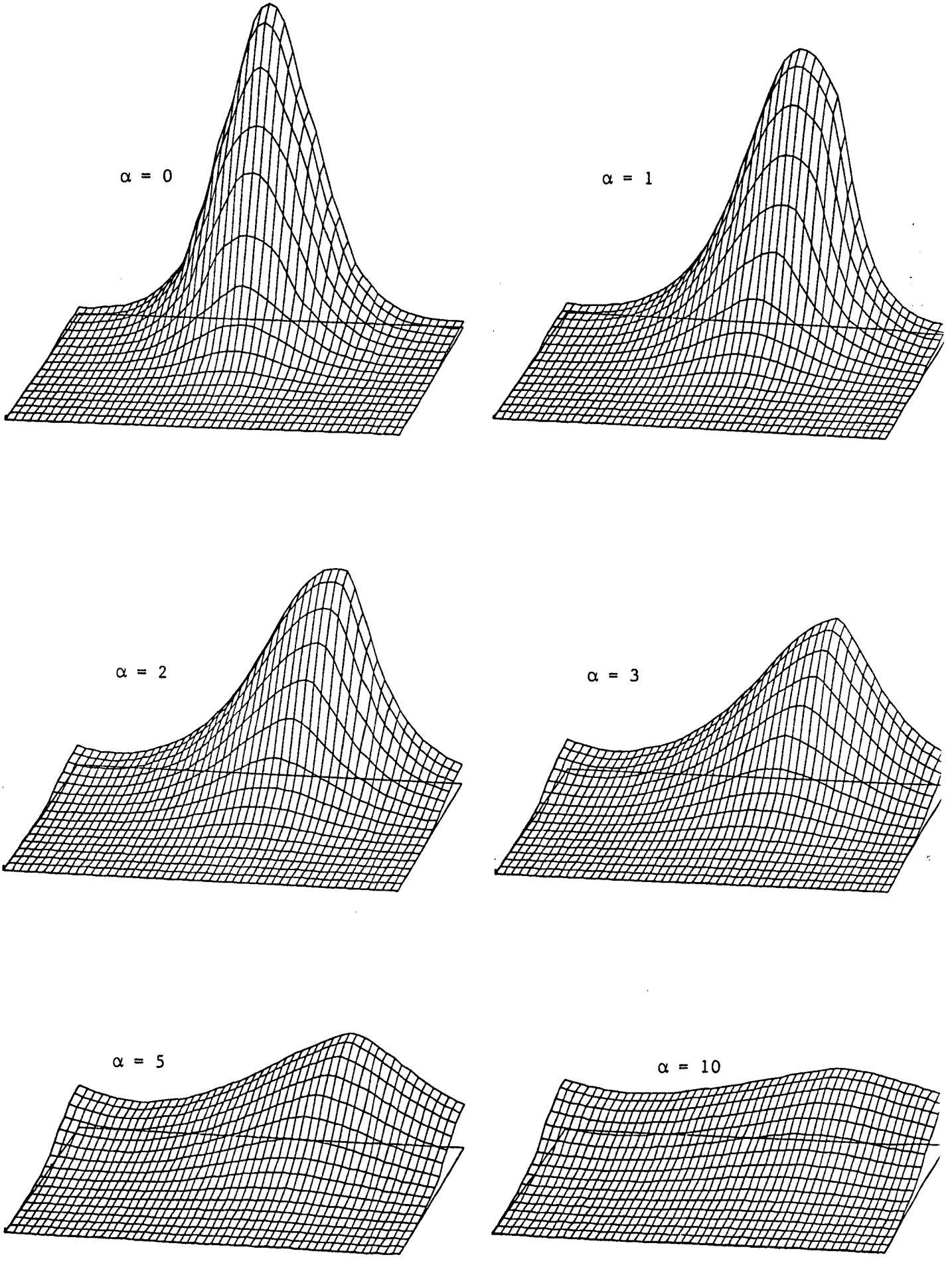


Figure 3 : Aspect of f for different electric fields.

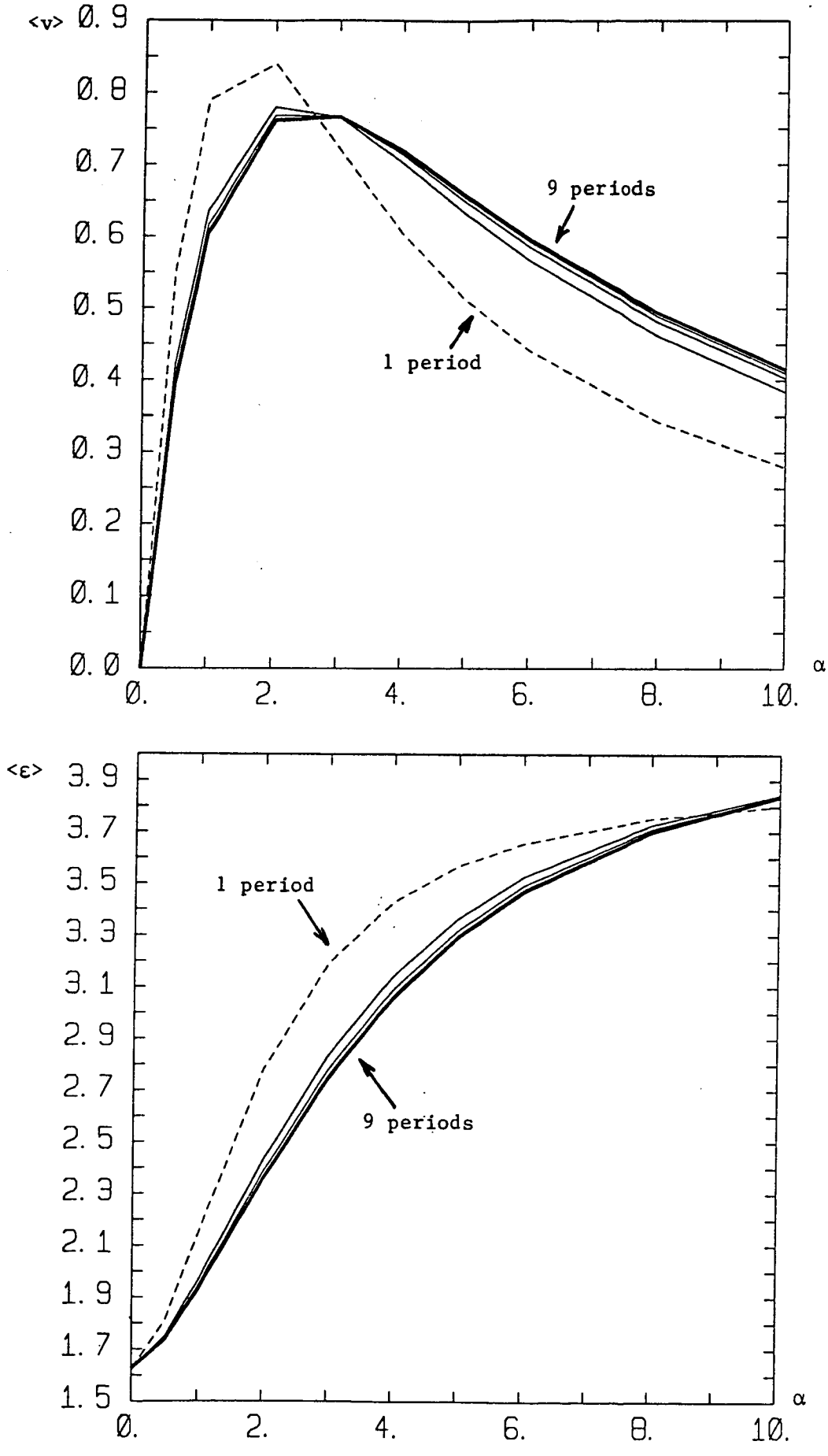


Figure 4 : Mean velocity and mean energy for $1, 3, 5, 7, 9$ periods.

4.3. The periodic evolution problem

The numerical study of the unsteady problem gives useful informations on the relaxation behavior of the solution towards its steady state.

The physical data are those of §4.2.1. The initial value of f is a Maxwellian distribution. The time steps are $\Delta t = 0.2$ for $\alpha = 3$ and $\Delta t = 0.05$ for $\alpha = 10$.

Using the upwind scheme, we observe the convergence in time towards the exact stationary solution of §4.2.1. Within three significant digits the values of $< v >$ and of $< \mathcal{E} >$ computed by the steady or by the unsteady solver are identical.

Moreover, for $\alpha = 10$, the unsteady solver yields a value $\lambda_1 = -0.24E - 4$ for the smallest eigenvalue of $T_h - S_h$ and the steady solver yields a multiplier value $\bar{\lambda} = -0.24E{-}9$. We observe therefore that we have $\bar{\lambda} = 0(\lambda_1^2)$ as predicted by the theory.

We have then used initial values of f with different energy levels. Figure 6 shows the influence of the initial distribution f_o on the transient behavior of the solution. When the energy of the initial distribution decreases, the amplitude and the number of oscillations increase. We also observe that this transient behavior is sharper and more oscillatory when the electric field increases. In fact, we observe, as predicted by the theory, that the frequency of these oscillations is proportional to the electric field (Fig. 5).

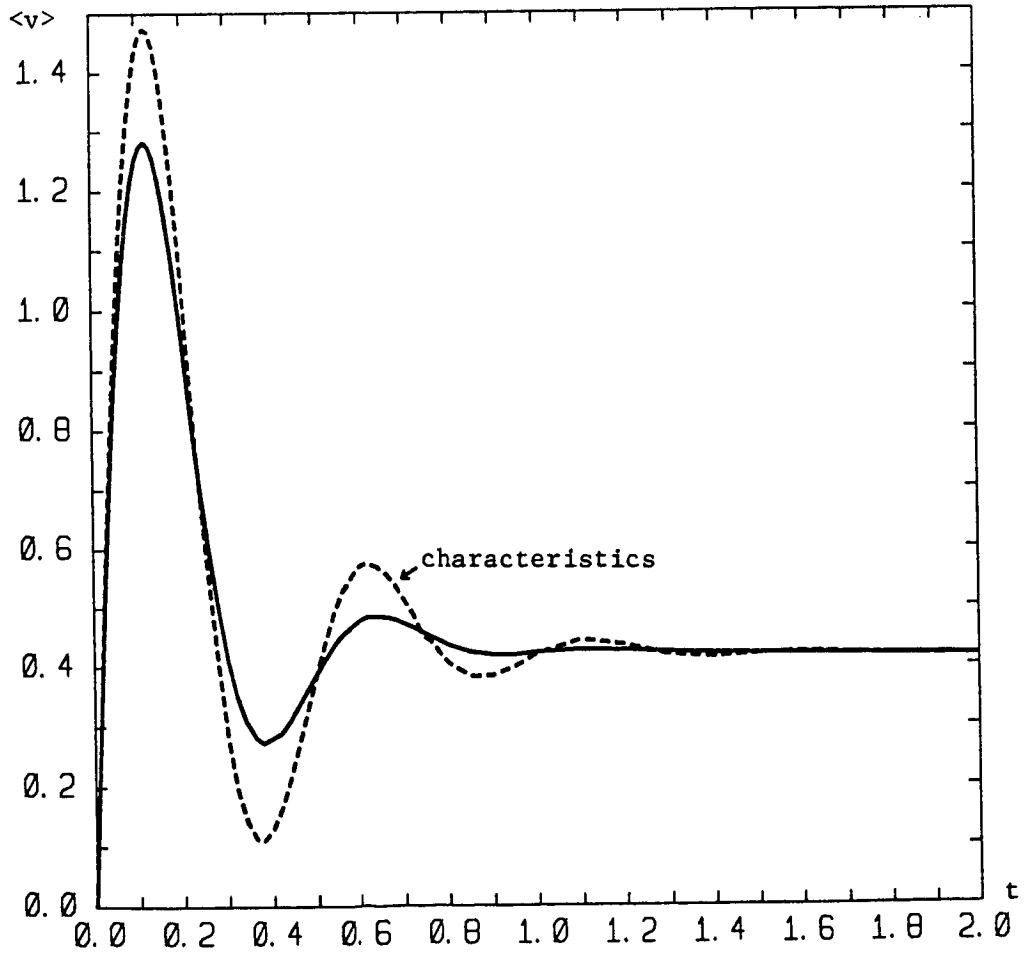
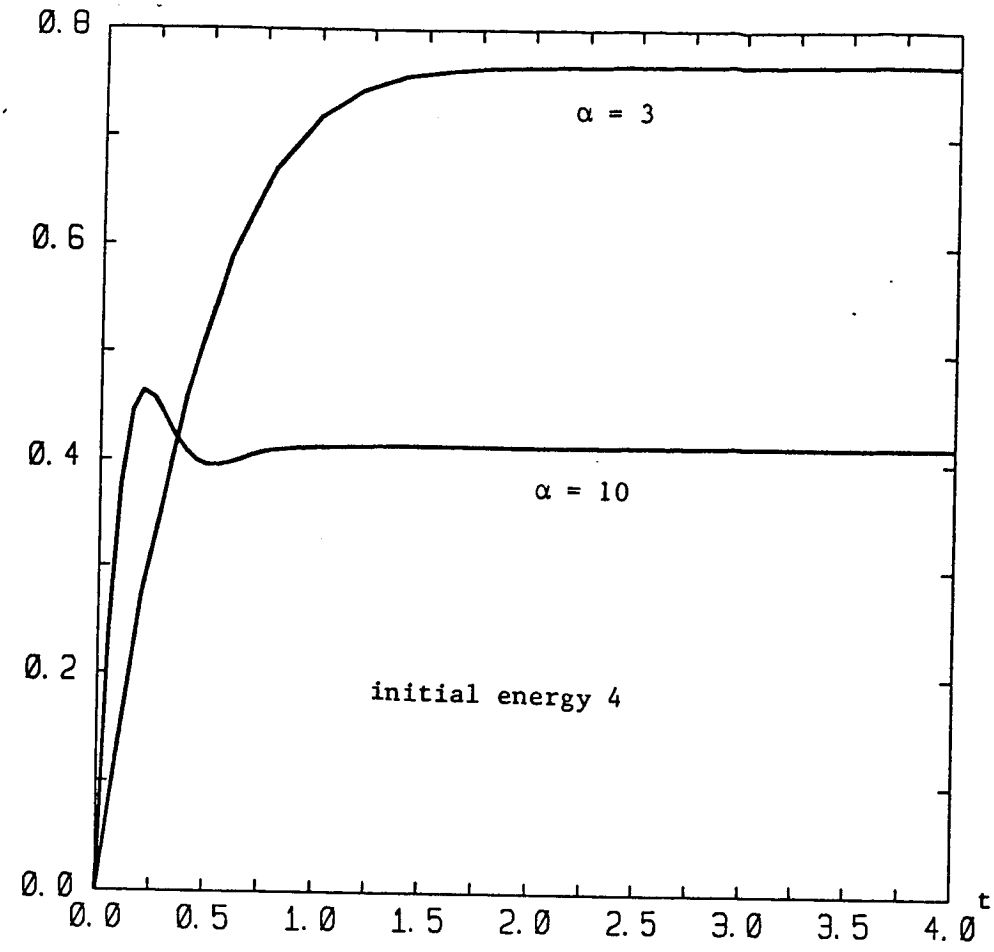


Figure 5 : Comparison between upwind scheme and characteristics.



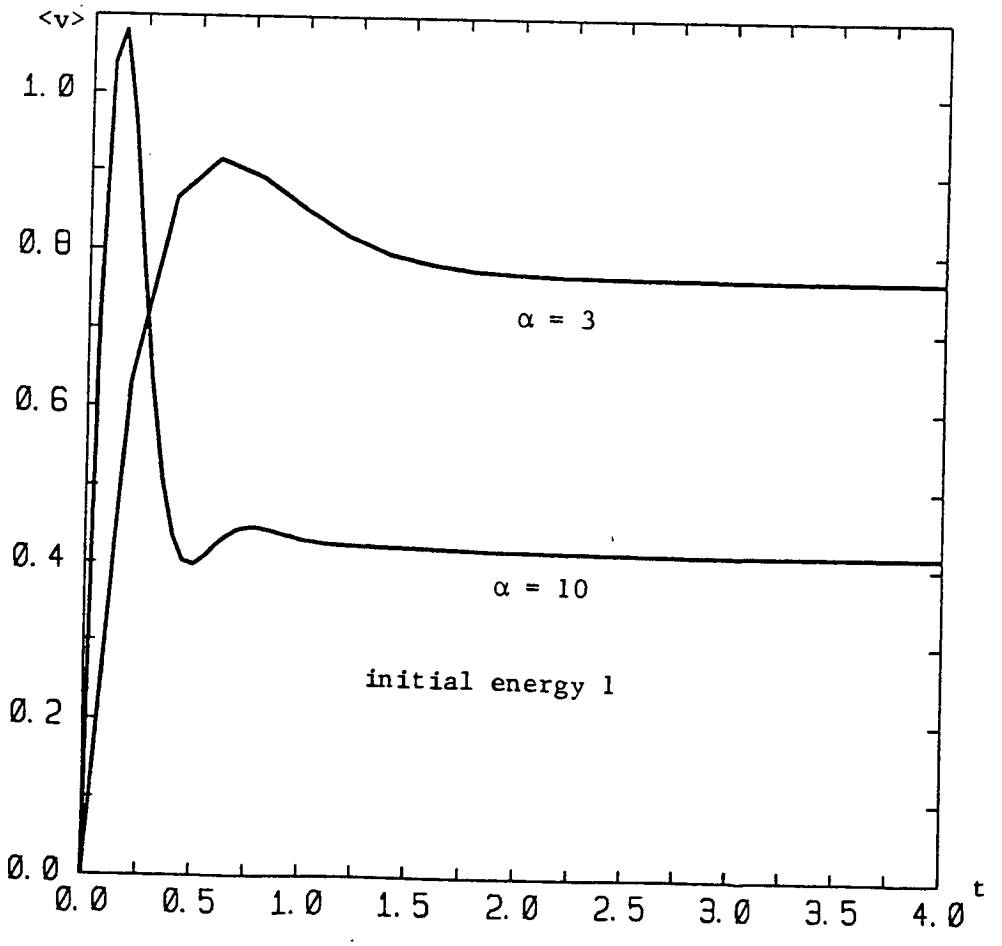


Figure 6 : Transient behavior of mean velocity for initial distributions with energy 1 and 4.

Therefore to get accurate results, at the numerical level, we have to use a time step which is inversely proportional to the electric field, leading to lengthy computations (15 mn of Cray 2 for $\alpha = 10$ with $\Delta t = 0.05$).

Figure 5 compares the results of our two time integration schemes (upwind or characteristics), for $\Delta t = 0.01, \alpha = 10$ and $f_o = exp(-0.8\varepsilon(k))$.

We indeed observe that the physical solution presents very large oscillations which are overshooted by the characteristics method and undershooted by the upwind scheme. Both solutions perfectly agree at the end.

4.4. The stationary unbounded problem

4.4.1. The model problem. Here we have :
$D_h = (-4,4) \times (0,4)$,
$h_z = h_r = 0.2$, (820 unknowns),
$\varepsilon(k) = |k|^2$,
$b_o = 0.4$ (reference cut-off parameter).

The corresponding results, with Dirichlet boundary conditions are summarized in Table 2. We observe that the quality of the numerical solution is low when $\alpha \geq 2$: $\int f$ is different from 1, the cost and $\bar{\lambda}$ increase. For large values of α, we get a discrete steady solution which is no longer compatible with the imposed boundary conditions.

Figure 7 shows the changes in the solution f when the results deteriorate.

α	<v>	<ε>	$\bar{\lambda}$	nit	cost	$\int f$
0	0	1.521	0.82E-8	73	0.32E-14	1.0000
0.5	0.279	1.773	0.11E-6	55	0.14E-12	1.0000
1	0.507	2.588	0.62E-5	45	0.57E-9	0.9991
2	0.878	5.476	0.13E-3	38	0.26E-6	0.9814
3	0.991	7.368	0.33E-3	36	0.19E-5	0.9512
4	0.952	8.409	0.51E-3	35	0.49E-5	0.9259
5	0.859	9.084	0.63E-3	35	0.82E-5	0.9089
6	0.757	9.581	0.71E-3	35	0.11E-4	0.8988
8	0.581	10.29	0.77E-3	37	0.17E-4	0.8911
10	0.454	10.78	0.78E-3	39	0.20E-4	0.8911

Table 2

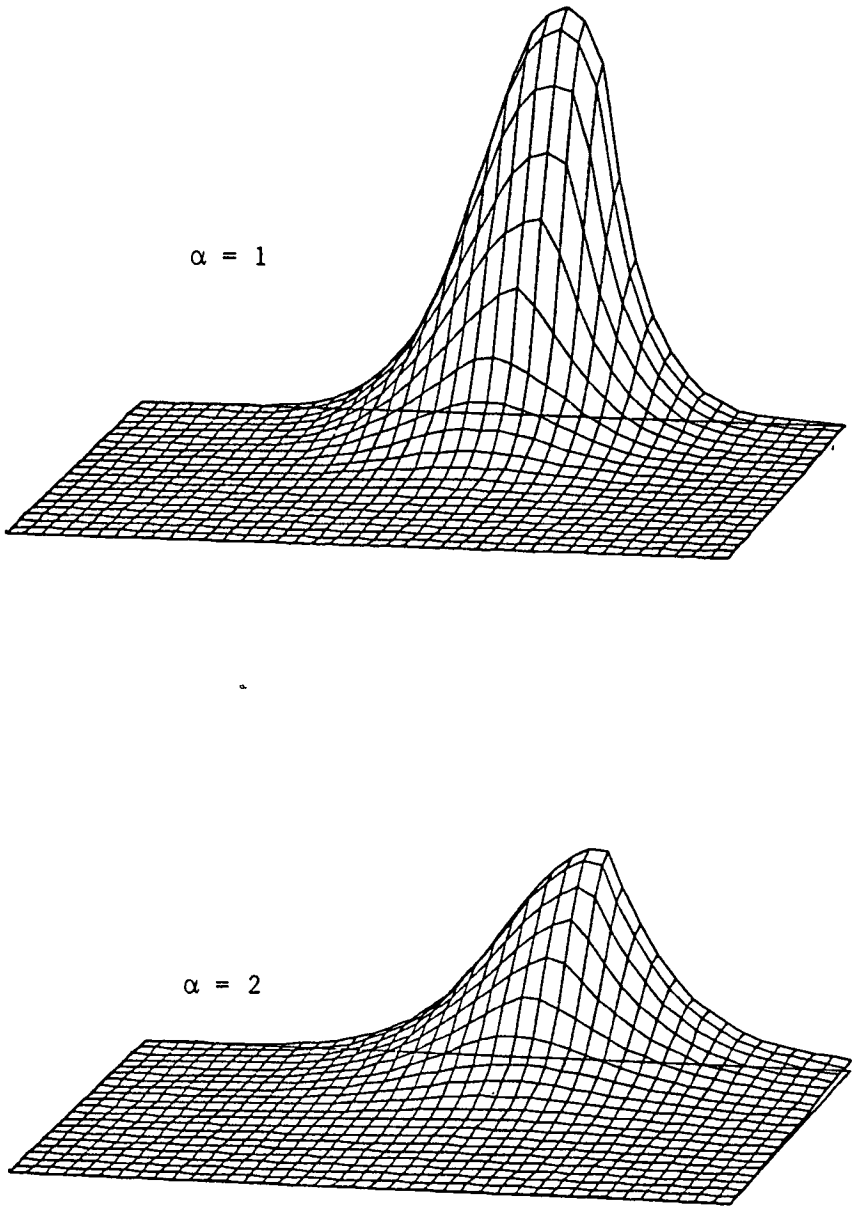


Figure 7: Aspect of f for boundary Dirichlet conditions.

4.4.2. Larger domain

We consider the same model problem, but set on the larger domain $D_h = (-8, 8) \times (0, 4)$. The results of Table 3 show the same deterioration when α gets larger than 2. On the other hand, for smaller values of α, the results are very similar to the previous ones. However, the computing time is now much larger because both the number of variables and the number of iterations increase. In summary, using a larger domain did not bring any improvement.

4.4.3. Changing the energy

We again consider the same model problem, still set on the domain $D_h = (-8,8) \times (0,4)$ but now we use an energy curve which is supposed to be more realistic for large wave vectors and which is given by

$$\varepsilon(k) = m^*|k|^2 + \frac{1}{2}\varepsilon_g[(1 + 4\frac{|k|^2}{\varepsilon_g}(1-m^*))^{\frac{1}{2}} - 1].$$

Above m^* is the effective mass and ε_g is a parameter which monitors the loss of parabolicity of the energy curve. This new energy curve is smaller for large values of $|k|$ and thus is more realistic when dealing with large domain and with Dirichlet boundary conditions. We indeed observe in Table 4 that this new energy now leads to acceptable numerical results for $\alpha = 2$.

4.4.4. Using periodic boundary conditions

We still consider the model problem of §4.4.1., but we now impose periodic boundary conditions on f. This change of boundary conditions has no effect when $\alpha \leq 1$ (Table 5). For larger values of α, the results are now quite good from the numerical point of view (lost cost, low value of $\bar{\lambda}$, $\int f \approx 1$) but they differ from those of the Dirichlet case and their physical validity remains questionable.

4.4.5. The unsteady approach

The data are still those of §4.4.1., but we now consider the evolution problem with $f_o = exp(-\varepsilon(k))$, with $\Delta t = 0.2$ for $\alpha = 2$ and $\Delta t = 0.05$ for $\alpha = 10$, and with Dirichlet boundary conditions.

By opposition to the periodic case, we have here to normalize f at each time step otherwise the value of $\int f$ will rapidly decrease as time grows. This normalization amounts to multiply f^n by a constant K in order to achieve $\int f = 1$. The value of this constant K is in fact related to the smallest eigenvalue λ_1 of the operator $T_h - S_h$ through the relation

$$\lambda_1 = (K-1)/\Delta t.$$

Figure 8 shows the aspect of the curve $< v > (t)$ for $\alpha = 2$ and $\alpha = 10$. Figure 9 shows the evolution of λ_1 as function of α : when $\alpha > 1$, this value is no longer negligible which means that then we do not have a true discrete steady solution.

On Figure 10, we finally compare the steady and the unsteady approach with Dirichlet boundary conditions by representing the curves $< v >_{(t=\infty)} - < v >_{steady}$ and $< \mathcal{E} >_{(t=\infty)} - < \mathcal{E} >_{steady}$ as functions of α. There also, these curves deviate from zero when $\alpha > 1$ which confirms the lack of discrete steady solution in these situations. Here, there is no discrete solution because, due to the Dirichlet condition, the discretization scheme is not conservative. Then the steady and the unsteady computations lead to two different pseudosolutions as indicated by a simple spectral analysis.

α	<v>	<ε>	$\bar{\lambda}$	nit	cost	$\int f$
0	0	1.521	0.23E-8	132	0.33E-14	1.0001
0.5	0.280	1.785	0.17E-7	95	0.14E-13	0.9999
1	0.582	3.284	0.23E-5	78	0.19E-9	0.9994
2	1.619	12.155	0.60E-4	61	0.12E-6	0.9851
3	2.176	17.7	0.16E-3	56	0.81E-6	0.9611
4	2.332	20.12	0.26E-3	50	0.20E-5	0.9389
5	2.319	21.32	0.34E-3	47	0.35E-5	0.92

Table 3

α	<v>	<ε>	$\bar{\lambda}$	nit	cost	$\int f$
0	0	1.576	-0.65E-9	115	0.23E-14	1.0000
0.5	0.248	1.788	-0.17E-8	93	0.63E-14	1.0000
1	0.440	2.468	0.32E-6	79	0.26E-11	0.9998
2	0.906	7.284	0.28E-4	61	0.20E-7	0.9936
3	1.231	11.84	0.10E-3	53	0.29E-6	0.9760
4	1.348	14.05	0.19E-3	49	0.94E-6	0.9565
5	1.367	15.14	0.28E-3	44	0.19E-5	0.9387

Table 4

α	<v>	<ε>	$\bar{\lambda}$	nit	cost	$\int f$
0	0	1.520	0.47E-8	76	0.22E-14	1.0000
0.5	0.279	1.774	-0.19E-8	53	0.89E-14	1.0000
1	0.492	2.656	-0.25E-8	45	0.26E-14	1.0000
2	0.645	6.310	-0.80E-9	33	0.21E-14	1.0000
3	0.548	8.613	-0.27E-10	28	0.87E-15	1.0000
4	0.445	9.642	-0.26E-9	25	0.19E-15	1.0000
5	0.370	10.15	-0.19E-9	25	0.35E-16	1.0000

Table 5

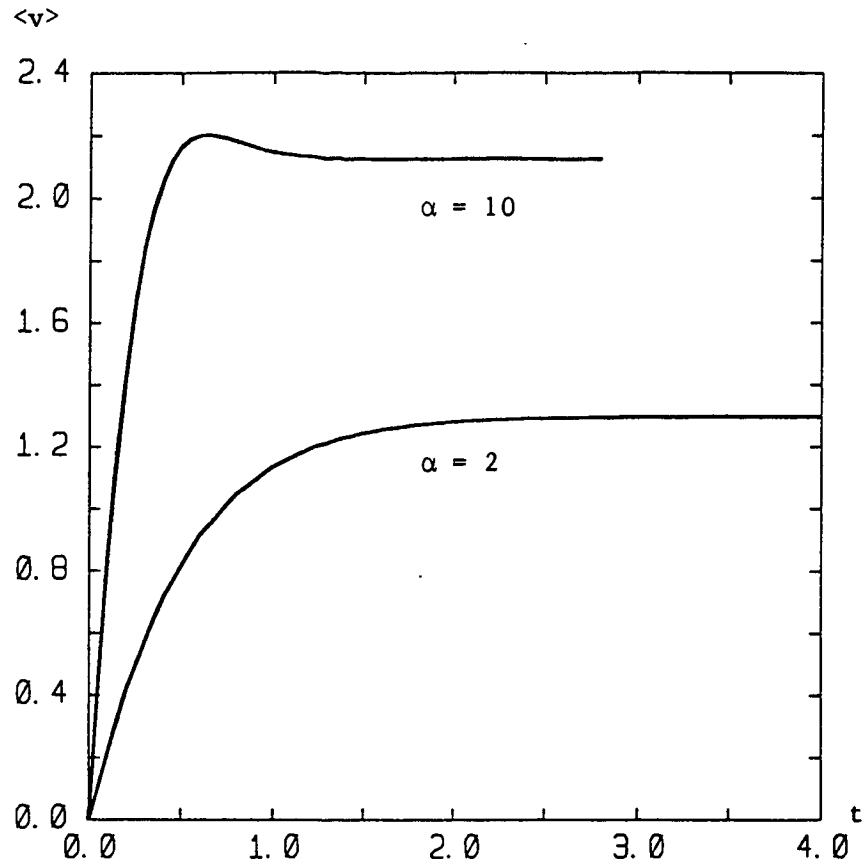


Figure 8 : Mean velocity versus time.

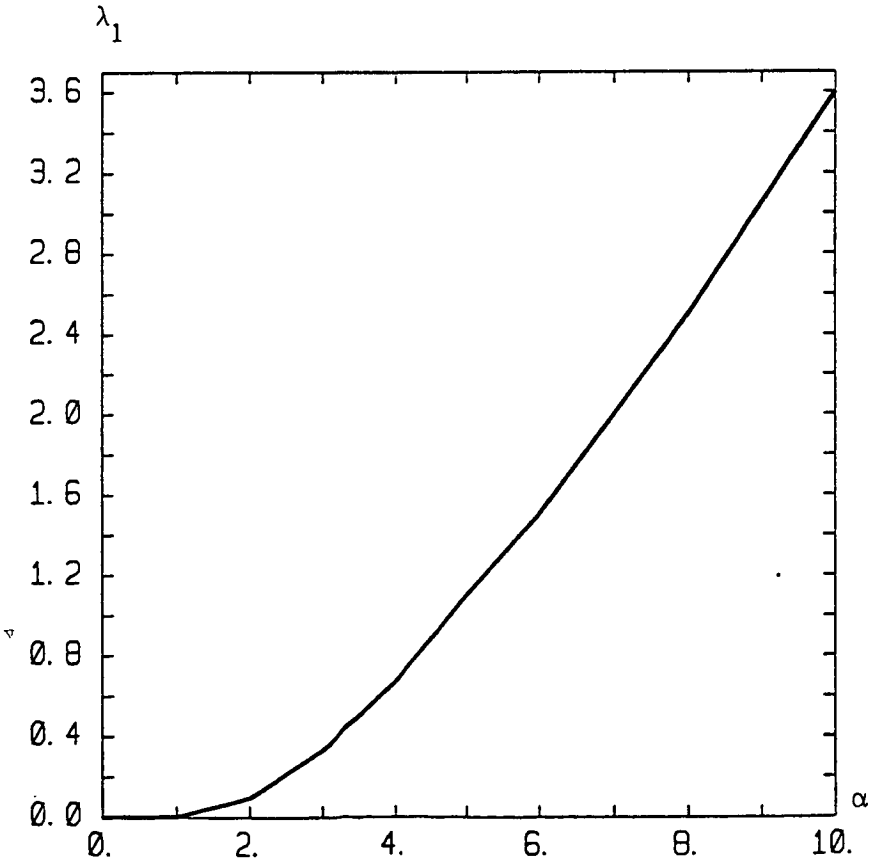


Figure 9 : Smallest eigenvalue of the operator $T_h - S_h$

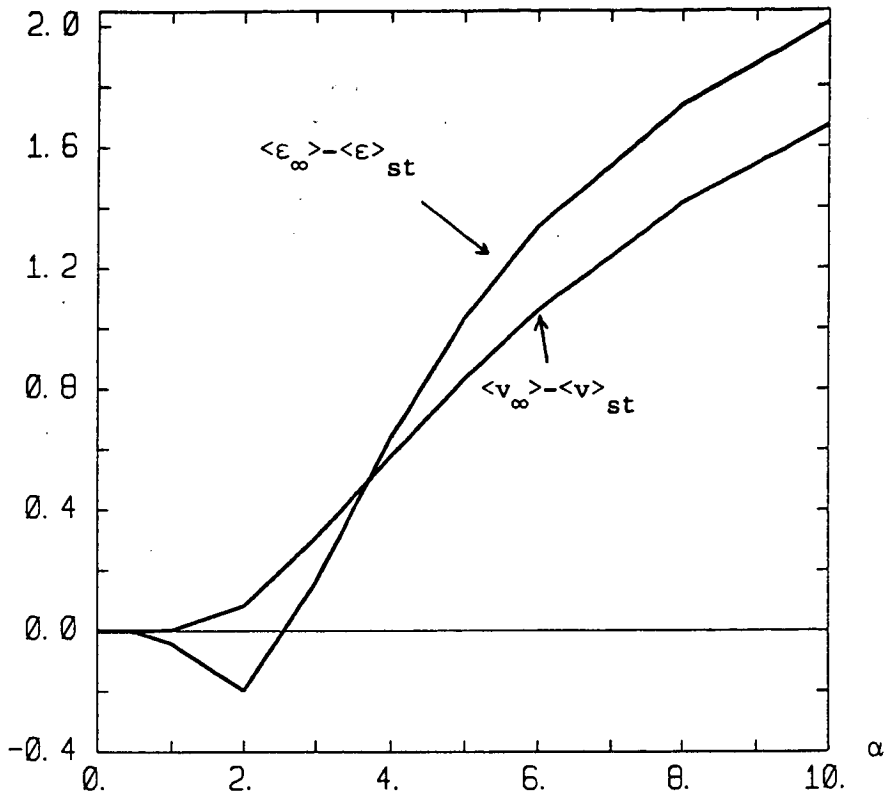


Figure 10: Comparison between the steady and the unsteady approach.

4.4.6. Conclusions on the Dirichlet problem

The three numerical approaches that we have used (steady Dirichlet, steady periodic, unsteady Dirichlet) to simulate the unbounded problem lead to two types of results :

- for $\alpha \leq 1$, all the results are consistent and of good numerical quality ;
- for $\alpha > 1$, the results are sensitive to the choice of boundary conditions and of solver. Moreover, the numerical quality of these results are poor when using Dirichlet boundary conditions, which corresponds to the fact that for these boundary conditions and for these values of α, there is no acceptable discrete steady solution ([7]).

5. Final comments

The combined use of upwind Finite Difference approximations and of least squares solution techniques has proved to be an efficient way of computing the steady solutions of the linear semiconductor Boltzmann equation.

In this process, the experience shows that one must be extremely cautious in the following operations :

i) manipulation of indices in the computation of the different integrals ;
ii) conservative calculation of the scattering out terms ;
iii) accurate computation of the gradient of the cost function ;
iv) use of physically compatible boundary conditions.

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